United States Environmental Protection Agency

NERL 2003

Office of Research and Development
National Exposure Research Laboratory

Building a Scientific Foundation for Sound Environmental Decisions

Computational Toxicology

On September 29–30, the EPA's ORD hosted a workshop on computational toxicology at the EPA Campus in Research Triangle Park, North Carolina. Participants discussed ways to fully utilize modern computing, chemistry, and molecular biology to develop predictive models of toxicity that improve quantitative risk assessments and reduce uncertainties in the source-to-outcome continuum. The workshop included presentations by EPA scientists that described the development of a research program within the Agency on computational toxicology.

Participants heard presentations from other federal agencies, academia, and outside research organizations about related goals and examples of computational approaches. In breakout sessions, participants envisioned the impact of computational toxicology on prioritization of chemicals for testing and improving quantitative risk assessment. Details will be posted at www.epa.gov/comptox/.

This year an ORD-wide steering committee has been developing a framework for a future initiative in computational toxicology. The steering committee, led by NHEERL's **Bob Kavlock**, includes NERL contributors **Eric Weber** and **Tim Collette (ERD)**, **Jerry Blancato (HEASD)**, and **Greg Toth (EERD)**. Toth is the Laboratory's computational toxicology program manager and **Kate Smith (EERD Director)** is NERL's lead.

Contact: Greg Toth
NERL-Cincinnati Ecological Exposure Research Division
(513) 569-7242

ORD's Epidemiological Study of Beaches Underway

An important part of EPA's Action Plan for Beaches and Recreational Waters is to improve our understanding of the link between water contaminants, swimming at the beach, and public health. To help us understand the link, NHEERL and NERL scientists are conducting an epidemiological study during the summer months from 2003 to 2005 at nine fresh and salt water beaches.

The epidemiological study is going to assist with development and evaluation of new-generation water quality tests for microbial contamina-

The EPA is studying water quality at beaches.

December 2003
Volume 6
Issue 2

tion that would provide **same-day results within two hours**, rather than the standard 24 to 48 hours. The study involves new water sampling protocols, coupled with interviews of approximately 5,000 families at two beaches in Indiana and Ohio during the summer of 2003. Families were interviewed on the beach about a variety of activities, including swimming. Ten to twelve days later, EPA researchers contacted the families to ask about their health in order to correlate indicators of poor water quality with reported adverse health effects.

On August 2, the first day of the study, NERL's **Al Dufour** joined **Paul Gilman**, EPA Science Advisor and Assistant Administrator for Research and Development, and U.S. Senator **George V. Voinovich** of Ohio for a press conference at Huntington Beach to talk about the importance of the research. "Swimming in water of poor quality can be a significant cause of stomach, respiratory, eye and ear illnesses in the summer time. Our goals are to prevent those illnesses and improve the quality of the water for recreation. EPA's science is providing the critical information that health officials and beach managers need to make decisions that protect the public health," said Gilman. "This important field research could not be done without the support of the community, and we greatly appreciate the contributions of the Cleveland Metroparks, Cuyahoga County Health Board and the citizens who agree to participate in this study. It also requires the support of Congress. Voinovich is a champion of using sound science to protect human health and the environment, and he continues to play a major role in restoring the Great Lakes to their natural vitality."

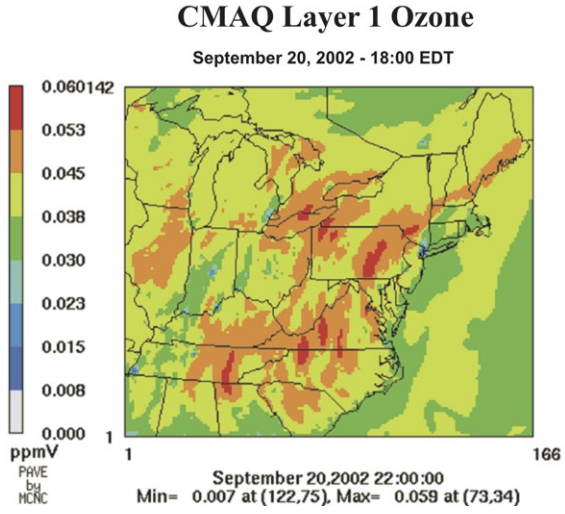
Contact: Alfred Dufour
NERL-Cincinnati
Microbiological and Chemical Exposure Assessment Research Division
(513) 569-7330

Community Multiscale Air Quality (CMAQ) Model — New Version

CMAQ, the numerical air quality simulation model developed by NERL and used by OAQPS, states, and others responsible for air quality planning and management, simulates tropospheric ozone, fine particles ($PM_{2.5}$), visibility, and acid deposition over continental through urban scales. During the last year, emphasis has been on refining the capabilities for simulating fine particles because the 2002 version showed considerable overestimates of nitrate and organic particles. Nitrate was found to be most severely overestimated during wintertime conditions. Thus, it was clear that improvements were necessary.

Scientists scrutinized the physical and chemical processes responsible for the production of nitrate in the CMAQ model and isolated several for improvement, one of which was the deposition of ammonia gas to a frozen ground surface during winter. (Ammonia is an important precursor gas to the chemical production of nitrate particles.) Model enhancements included an increase in ammonia deposition, leading to a decrease in nitrate production.

Scientists also studied the atmospheric chemistry. The reaction of N_2O_5 with water on the surface of existing particles was found to be an important source of nitric acid, another precursor of nitrate particles. Recent studies of this reaction cited in the literature show a much lower probability of this reaction occurring than was shown in earlier studies. In response, changes in the CMAQ model were implemented which reduced nitrate particle concentrations by **25–65%** over the continental U.S. model domain, bringing them closer to observed ambient levels.



Additionally, scientists examined the process of partitioning the organic material between gases and particles. CMAQ's earlier versions included a gas-to-particle pathway for organic material, allowing organic particles to grow in the atmosphere. However, the reverse pathway, from particles back to gas, is also significant and was added to the CMAQ model during recent testing. The reverse pathway for organic partitioning resulted in the lowering of secondary organic particle concentrations by 60–70% in the CMAQ model simulations, which compare more favorably with observed concentration levels.

Last but not least, efforts continue toward making the CMAQ model run more efficiently on typical user computer platforms. Recent tests of the CMAQ model on a 12-processor Linux cluster showed a **24-hour simulation running in less than two hours of real time**. Further efficiency improvements are anticipated over the coming year. The latest version of the CMAQ model is available from the Community Modeling and Analysis System (CMAS) web site: www.cmascenter.org.

Contact: Ken Schere
NERL-RTP Atmospheric Modeling Division
(919) 541-3795

SHEDS Predicts Pesticide Exposure

The Stochastic Human Exposure and Dose Simulation (SHEDS) model for pesticides (SHEDS-Pesticides) increases the Agency's understanding of human exposures and doses to multimedia, multipathway pollutants. It is a physically-based, probabilistic computer model that predicts exposures and doses incurred by selected groups of people associated with contamination from eating, drinking water, inhaling air, coming in contact with surface residues, or ingesting residues from hand- or object-to-mouth activities. To do this, SHEDS-Pesticides combines information on pesticide usage, human activity data (from time/activity diary surveys and videography studies), environmental residues and concentrations, and exposure and dose factors using one- or two-stage Monte Carlo probabilistic sampling methods. This research will help answer the following questions:

CCA-treated wood is used on playsets & decks.

- What is the population distribution of exposure for a given cohort for existing scenarios or for proposed exposure reduction scenarios?
- What is the uncertainty associated with different percentiles of exposure for a population?
- What is the intensity, duration, frequency, and timing of exposures from different routes?
- What are the most critical media, routes, pathways, and factors contributing to exposures?
- How can exposures be most effectively reduced?
- What additional human exposure measurements are needed to reduce uncertainty in population estimates?
- How do modeled estimates compare to real-world data?

Although SHEDS-Pesticides has been developed as a source-to-dose model, the concentration-to-exposure module has been the primary focus of development and relatively simple modules are currently incorporated for source-to-concentration and exposure-to-dose estimation.

A scenario-specific model, SHEDS-Wood, was developed by NERL at the request of the Agency's OPP to focus on children's exposure and dose to arsenic and chromium from chromated copper arsenate (CCA)-treated wood on playsets and decks. The results were presented successfully to OPP's Federal Insecticide, Fungicide and Rodenticide Act (FIFRA) Science Advisory Panel (SAP) last summer. Currently, we are refining the SHEDS-Wood model to incorporate new data and to address SAP comments. The information will be used as part of OPP's public health risk assessment to be presented to the SAP in 2003 as a final technical report. In the interim, scientists at the EPA are completing the modeling runs and producing the reports needed for the next SAP meeting. The SHEDS-Wood model will form the basis of the exposure

and dose assessments that OPP will use to calculate cancer and non-cancer risks for children who come in contact with CCA-treated playsets and decks. The documentation, code, interface, and a journal article on the SHEDS-Wood assessment of CCA-treated wood will be completed in 2004.

Contact: Valerie Zatarian
NERL-RTP Human Exposure and Atmospheric Sciences Division
(617) 918-1541

Weaver — He's a Smooth Calculator

In most households, a calculator is used to balance the checkbook. However, **Jim Weaver**, of NERL's ERD uses more than 30 calculators to assess the transport of subsurface contaminants. At work Weaver considers himself not only an engineer, but a public servant and a teacher as well. He attributes his perspective on public service to his alma mater, the University of Texas, Austin, where he received his Ph.D. in Civil Engineering in 1988. "Where I went to school, research, consulting, and teaching were a three-pronged approach for educating people and advancing scientific knowledge," he says. Weaver exudes a genuine enthusiasm for helping people, especially environmental professionals in EPA's regional offices and state agencies.

Jim Weaver

In 1994, while Weaver was working at EPA's NRMRL in Ada, Oklahoma, he also taught classes on groundwater modeling. At one of his workshops, a State of New York employee asked him for help with interpretation of a rich data set depicting MTBE from leaking underground storage tanks (LUST). Weaver welcomed the opportunity to help and to this day, continues EPA's nine-year collaboration with them on subsurface contamination.

In 1996, Weaver joined NERL-Athens where he developed a new course on modeling subsurface contamination from petroleum hydrocarbons to help EPA Region 4. Others were eager to have access to guidance and tools for the ever-increasing problem of LUST, and Weaver found himself teaching the course to people in more than 20 states nationwide.

As demands for his time grew, Weaver decided to 'prepackage' the principles of groundwater flow by developing a suite of calculators called "OnSite" and to make them available from the web. OnSite provides methods and data for common calculations meaningful to a variety of users for assessing impacts from subsurface contamination. Parameter estimates are also included for the convenience of those with experience, the education of those with less experience, and because of their potential to provide consistency among a diverse user community.

Since their beginning, the OnSite calculators have come a long way. More than 30 calculators cover parameter estimates, simple transport models, unit conversions, and scientific demonstrations like Darcy flow in a laboratory column. Some of the concepts contained in the OnSite calculators have come directly from interactions with the states, including plume diving and borehole concentration averaging that were a result of the interaction with the State of New York on the aforementioned MTBE sites.

Knowledgeable groundwater experts have said that because of their high level of confidence in the OnSite calculators — prepackaged formulas and data — they no longer have to refer back to written texts. Today, state environmental agency staff are referring their consultants to the web site (www.epa.gov/athens/onsite), which receives about 18,000 hits per month.

"My work helps with their problems. By offering these calculators, I've learned the real problems practitioners are dealing with," says Weaver. "You get back more than what you give people. Someone I work with characterized it as a labor of love. And that's about right."

EPA and NOAA Join Forces in Atmospheric Modeling Research and Air Quality Forecasts

In a ceremony in Washington, D.C., then-EPA Administrator **Christine T. Whitman** and Deputy Secretary of Commerce **Samuel W. Bodman** signed an MOU to reaffirm a long-standing collaboration on atmospheric sciences research and an MOA to develop and implement a **national air quality forecasting system**. The two agencies are joining forces to enhance research in air quality modeling and atmospheric measurements for developing a consistent, national numerical air quality model for short-term forecasts for ozone, fine particulate matter, and visibility.

"An improved air quality forecast can mean a higher quality of life for many Americans, especially those most vulnerable to the effects of ozone," said Bodman. Air pollution control agencies across the country will use the new national prediction model to supplement their forecasts of local air quality indices.

The partnership between EPA and NOAA dates back to 1955, when a handful of Weather Bureau meteorologists were assigned to the Public Health Service to work on air pollution problems. Today, more than 50 atmospheric scientists are on assignment at EPA where they conduct research in air pollution meteorology, atmospheric modeling, and air quality data analysis and management.

Led by **S. T. Rao**, the NERL's AMD develops air quality models for use by EPA in its regulatory decision making, including the Community Multiscale Air Quality (CMAQ) model (featured on page 2). The MOA brings together the National Weather Service and AMD in the development of an integrated meteorological-chemical transport model for simulating ambient air quality of the continental U.S. Work continues into the fall of 2004, when EPA and NOAA will produce a numerical air quality model that provides daily forecasts for ozone in the northeastern U.S.

The EPA-NOAA partnership will pay benefits well into the future. Within five years, the system for ozone will be deployed nationwide; within ten years, the model is expected to be used in forecasting PM in four-day increments. Citizens at the state and local level will benefit because their local air quality management agencies will provide them with better and more timely air quality forecasts.

Contact: S. T. Rao
NERL-RTP Atmospheric Modeling Division
(919) 541-4542

NERL Scientists Participate in the ISEA Meeting

Larry Cupitt, NERL's Associate Director for Health, led a delegation of scientists to the annual International Society of Exposure Analysis/International Society of Environmental Epidemiology conference in Stresa, Italy (September 21–25, 2003). NERL participants are all members of the HEASD, including **Elaine Hubal** (Acting Associate Director for Human Exposure Modeling), **Haluk Ozkaynak** (Senior Science Advisor), **Curtis Dary** (Acting Chief, HEASD Exposure Dose Research Branch), **Thomas McCurdy, Marsha Morgan**, **Liu Shi, Jianping Xue**, **Lance Wallace**, and postdocs **Peter Egeghy** and **Rogelio Tornero-Velez**.

The International Society of Exposure Analysis (ISEA), a multi-disciplinary, international organization, is dedicated to advancing the science of exposure analysis for human populations and ecological systems. ISEA is the primary organization for EPA's exposure researchers and their counterparts. This year's agenda included tracks on risk management, methodological advances, and dietary, indoor, urban, rural, workday, and population exposures.

Contact: David Kryak
NERL-RTP Human Exposure and Atmospheric Sciences Division
(919) 541-2454